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Multiscale Thermohydrologic Model: Addressing Variability and Uncertainty at Yucca Mountain

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Introduction

Performance assessment and design evaluation require a modeling tool that simultaneously accounts for processes occurring at a scale of a few tens of centimeters around individual waste packages and emplacement drifts, and also on behavior at the scale of the mountain. Many processes and features must be considered, including non-isothermal, multiphase-flow in rock of variable saturation and thermal radiation in open cavities. Also, given the nature of the fractured rock at Yucca Mountain, a dual-permeability approach is needed to represent permeability. A monolithic numerical model with all these features requires too large a computational cost to be an effective simulation tool, one that is used to examine sensitivity to key model assumptions and parameters. We have developed a multi-scale modeling approach that effectively simulates 3D discrete-heat-source, mountain-scale thermohydrologic behavior at Yucca Mountain and captures the natural variability of the site consistent with what we know from site characterization and waste-package-to-waste-package variability in heat output. We describe this approach and present results examining the role of infiltration flux, the most important natural-system parameter with respect to how thermohydrologic behavior influences the performance of the repository.

A Multi-scale Modeling Approach

Conceptually, our approach is simple. We directly simulate thermohydrologic behavior for an "average" waste package in a 2D drift cross-section for a variety of heat-generation densities at many locations throughout the repository. In these simulations, we account for the flow of liquid and gas (water vapor and air) through variably-saturated fractured porous media with a dual-permeability representation of permeability. We also account for two-phase behavior (i.e., evaporation, boiling, condensation). We represent thermal conduction and convection in the rock and thermal conduction, convection and radiation in open drifts.

We then modify these 2D thermohydrologic model results with 3D thermal model results to account for 3D heat flow at the mountain scale and for 3D heat flow at the drift scale, which accounts for waste-package-to-waste-package variability in heat output. We assume that any mountain-scale movement of water and water vapor along the drift axes or between drifts can be neglected (i.e., all fluid flow is confined to 2D vertical cross section orthogonal to the drift axis, with no fluid flow across the vertical midplane in the rock pillar between the drifts). We also neglect changes in rock properties due to coupled thermohydrologic-chemical-mechanical processes and the effect of dissolved solutes on the thermohydrologic properties of water.

Sensitivity to geographic location in the repository reflects differences in local stratigraphy, overburden thickness, host-rock unit, and percolation flux. It also reflects differences in proximity to repository edges, which is important because a waste package at the edge of the repository will cool more quickly than one at the center. We assume that mountain-scale temperature variability is governed by conduction. This assumption, which preserves mountain-scale temperature variability, is equivalent to assuming that the primary modes of heat convection (the heat-pipe effect and buoyant gas-phase convection) have a negligible influence on temperature variability between the center of the repository and the edges.

Drift-scale variability in temperature along the drift axis will result from differences in heat output from individual waste packages. We assume that this variability is governed by thermal conduction in the host rock and in-drift components, and by thermal radiation in the open drift cavities. This assumption, which preserves drift-scale temperature variability, is equivalent to assuming heat convection has a negligible influence on temperature variability along the axis of the drift.

We represent all possible waste packages by four major types: civilian spent nuclear fuel from power-water-reactors (PWRs) and from boiling-water-reactor (BWRs), high-level waste (HLW) and defense spent nuclear fuel (DSNF). We consider a waste-package sequence resulting in eight unique waste packages (i.e., we distinguish between a BWR placed between a PWR and a HLW and a BWR placed between two PWRs).

To implement this multi-scale approach, we have developed a modeling methodology we call the Multiscale Thermohydrologic Model (MSTHM). The MSTHM consists of several major submodels of various scale, dimensionality, heat-source representation, and assumptions regarding both the heat transfer processes considered and the coupling of heat transfer to fluid flow. These submodels are all based on NUFT, a flexible multipurpose computer code for modeling non-isothermal, unsaturated fluid flow and transport in porous and fractured media[1].

The Multiscale Thermohydrologic Model consists of four submodels:

- **SMT** (Smeared-heat-source, Mountain-scale, Thermal-conduction) Submodel
- **LDTH** (Line-averaged-heat-source, Drift-scale, Thermohydrologic) Submodel
- **SDT** (Smeared-heat-source, Drift-scale, Thermal-conduction) Submodel

- **DDT** (Discrete-heat-source, Drift-scale, Thermal-conduction) Submodel

The LDTH submodel domain is a 2D drift cross-section extending from the ground surface to the water table. LDTH submodels are run for different locations spaced evenly throughout the repository area, and use the stratigraphy, overburden thickness, thermal boundary conditions, and infiltration fluxes appropriate for each location. SDT submodels, which are 1D vertical submodels, are run at the same locations as the LDTH submodels. Both submodels assume a heat-generation history of the entire waste inventory averaged over the total heated length of emplacement drifts in the repository.

The 3D SMT submodel accounts for the repository footprint in Yucca Mountain, allowing consideration of important thermal processes such as edge-cooling effects. This submodel assumes a heat-generation history of the entire waste inventory averaged over the heated footprint of the repository.

Output from the LDTH, SDT, and SMT submodels are integrated to create a 3D LMTH (Line-averaged-heat-source, Mountain-scale, Thermohydrologic) model.[2,3] The 3D DDT submodel is then used to further modify the LMTH model to account for waste-package-specific deviations from line-averaged behavior and for thermal radiation in drifts. The end result is a 3D DMTH (Discrete-heat-source, Mountain-scale, Thermohydrologic) model. The submodels are integrated with the Multiscale Thermohydrologic Abstraction Code (MSTHAC), shown schematically in Fig. 1.

The MSTHM calculates thermohydrologic variables in the fracture and matrix continuum at a variety of locations (e.g., drift wall, waste package, and various locations in the host rock surrounding the drift) for numerous repository locations (610 in the example presented here) and different waste packages, as a function of time. Thermohydrologic output variables include temperature, relative humidity, liquid-phase saturation, liquid-phase flux, gas-phase air-mass fraction, gas-phase pressure, capillary pressure, gas-phase flux (water vapor, air), and evaporation rate.

Sensitivity to Natural-System Uncertainty

The key natural-system uncertainty influencing thermohydrologic behavior is infiltration flux. To examine the influence of infiltration flux on repository thermohydrologic behavior, we simulated the YMP TSPA-SR design[4] (for three infiltration-flux cases. In all cases, infiltration fluxes vary spatially across the repository and increase significantly after 600 years, and then increase further after 2000 years. Results are shown in **Fig. 2**.

The spatial extent of boiling decreases with increasing infiltration flux (**Fig. 2a**). The low infiltration-flux case has a longer duration of rock dryout then either the mean or high infiltration-flux cases (**Figs. 2b**). The influence of infiltration flux on peak waste-package and drift-wall temperature is shown in **Figs. 2c and 2d**. Peak temperatures are highest for the low-infiltration case and lowest for the high-infiltration case. Peak temperatures are about 5°C higher for the low-flux case than the mean-flux case and about 5°C lower for the high-flux case than the mean-flux case.

The low infiltration-flux case results in a more persistent reduction in *RH* on waste packages than the mean and high flux cases, which show similar behavior (**Figs. 2e and 2f**). The mean and high flux cases have similar waste-package temperatures once an *RH* of 80% is attained on the waste packages, whereas the low flux case results in much lower temperatures. These results imply that there is an infiltration-flux threshold value above which *RH* reduction becomes significantly limited, and that the values for the mean case considered here approach this value for the TSPA-SR design. Further increases in infiltration flux have a diminishing effect on decreasing the duration of *RH* reduction.

Conclusions

We have demonstrated a uniquely powerful multi-scale modeling approach for examining thermohydrologic behavior at Yucca Mountain that captures both the variability of the natural system at the site, consistent with what we know from site characterization, as well as the variability of the heat output from the waste-package inventory. This approach is also unique because it captures the full dimensionality of thermohydrologic behavior in the emplacement drifts and near-field host rock, including both 3D drift-scale heat flow and 3D mountain-scale heat flow. Therefore, it captures the full spectrum of thermohydrologic environments in the drifts and in the near field for the waste-package inventory. This approach is a very useful tool for analyzing uncertainty in key model parameters and assumptions and for analyzing conceptual-model uncertainty (e.g., approximations for fracture-matrix interaction).

For the TSPA-SR repository design, we considered uncertainty in infiltration flux, which is the most important natural-system parameter with respect to how thermohydrologic behavior influences the performance of the repository. We found that peak temperatures, as well as the spatial extent and duration of boiling, decrease with increasing infiltration flux. The duration of reduced *RH* on waste packages also decreases with increasing infiltration flux. We also find that there is a threshold infiltration flux above which further increases in infiltration flux have a diminishing influence on decreasing these thermohydrologic variables.

References

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3. Civilian Radioactive Waste Management System, Multiscale Thermohydrologic Model, *Rep. ANL-EBS-MD-000049 REV 0*, TRW Environ. Safety Syst., Inc., Las Vegas, Nev., 2000.
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Figure Legends

Fig. 1 Schematic of the Multiscale Thermohydrologic Model (MSTHM), which consists of a family of four NUFT-based submodels of various scales, dimensionality, and processes, which are integrated with the Multiscale Thermohydrologic Abstraction Code (MSTHAC).

Fig. 2 Complementary cumulative distribution function (CCDF) plots showing the sensitivity of the TSPA-SR repository design to uncertainty in the infiltration flux.

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Fig. 1

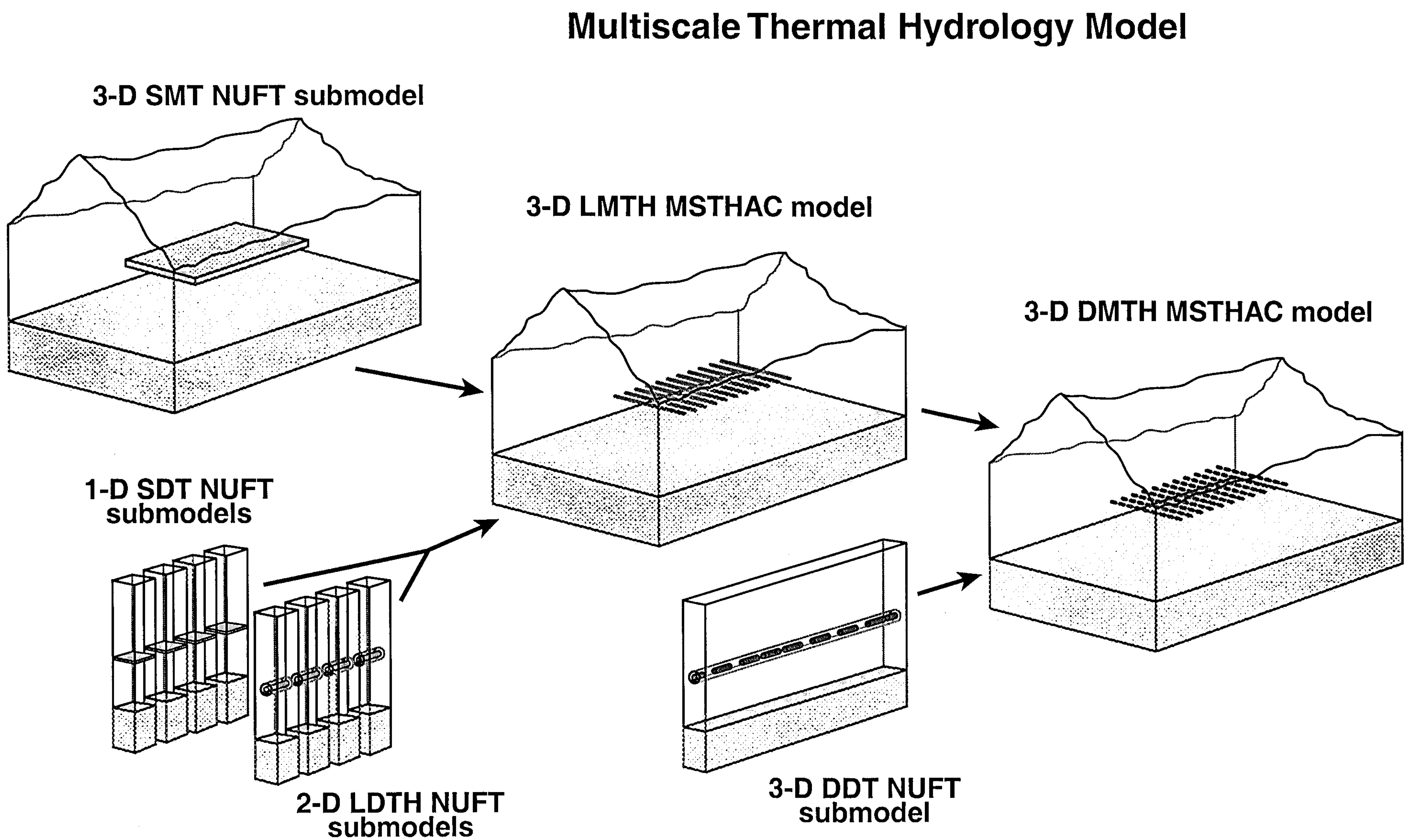
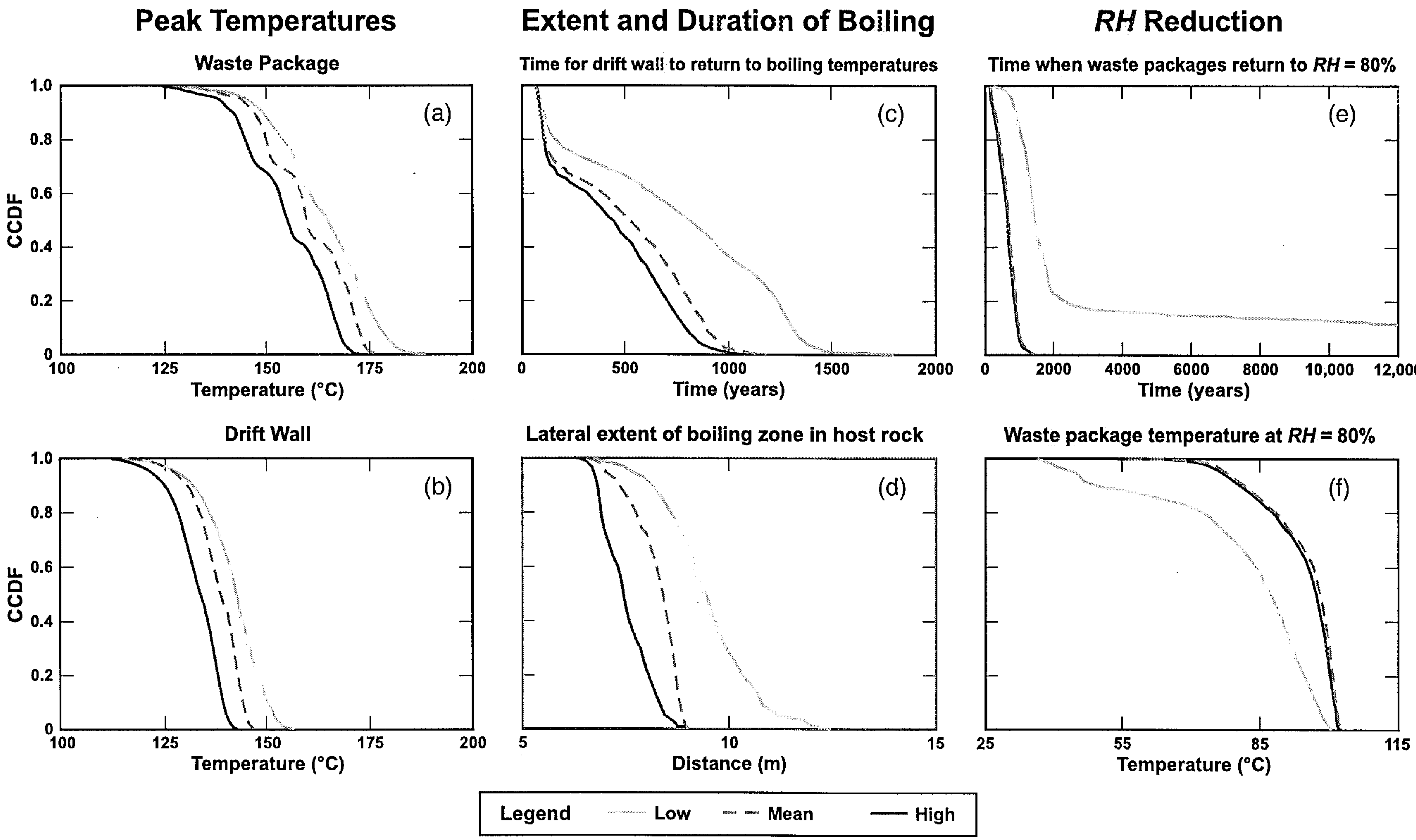

Multiscale Thermal Hydrology Model
3-D SMT NUFT submodel
3-D LMTH MSTHAC model
3-D DMTH MSTHAC model
1-D SDT NUFT submodels
2-D LDTH NUFT submodels
3-D DDT NUFT submodel

Fig. 2



Peak Temperatures
Extent and Duration of Boiling
RH Reduction
Waste Package
Time for drift wall to return to boiling temperatures
Time when waste packages return to RH = 80%
(a)
(c)
(e)
CCDF
Temperature (°C)
Time (years)
Time (years)
Drift Wall
Lateral extent of boiling zone in host rock
Waste package temperature at RH = 80%
(b)
(d)
(f)
Distance (m)
Temperature (°C)
Legend
Low
Mean
High

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